alpha-Humalene
6753-98-6 | DTXSID30858793

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 2.58 days

Global applicability domain: Outside

Local applicability domain index: 4.57e-01

Confidence level: 8.92e-01

Nearest Neighbors from the Training Set

Image not found
3-Methylindene
Measured: 12.5
Predicted: 2.76

Image not found
1H-Indene, 2-methyl-
Measured: 12.5
Predicted: 2.48

Image not found
4-Methylindan
Measured: 4.93
Predicted: 2.31

Image not found
Indene
Measured: 12.5
Predicted: 7.90

Image not found
5-Methylindan
Measured: 4.93
Predicted: 2.25